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"GAP" STATE OF THE BAC HAMILTONIAN FOR REPULSIVE INTERACTIONS

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For attractive interactions between particles the "energy gap" equation stemming from the reduced Hamiltonian of the BCS theory has two familiar solutions.(1) One solution yields a gap and leads to the correlated ground state. The other solution yields no gap and leads to an uncorrelated state which is identical to the ground state in the absence of interaction. This state has a higher energy than the correlated ground state and corresponds to an excitation of the correlated state. This excitation can be described as the "breaking" or "ionization" of each of the infinite number of condensed electron pairs that make up the ground state, the energy required to break a pair being twice the energy of the gap. With attractive interactions, then, the "gap" state -- the state with correlations -- is the stable state.

For repulsive interactions between particles a correlated state can again be obtained, but it is no longer the stable state, the ground state now being the normal state. One now finds that to break a correlated pair no longer takes energy, but rather gives energy. Thus, even though one can obtain Cooper pairs for repulsive interactions(2), and even though these pairs can be condensed into a correlated state, such a state is not stable.

Before exhibiting the correlated state that arises from repulsive interactions, we first show that for such interactions it is the normal state that must be the ground state.

The Hamiltonian is, $H_o + H_{int}$:

$$\sum_k \left[\varepsilon_k^\circ - \mu\right]\left[C_{k\uparrow}^+ C_{k\uparrow} + C_{-k\downarrow}^+ C_{-k\downarrow}\right]$$

$$+ \frac{1}{V} \sum_{\mu - \delta \leq \varepsilon^\circ(\kappa), \varepsilon^\circ(k) \leq \mu + \delta} A(k)A(\kappa)C_{k\uparrow}^+ C_{-k\downarrow}^+ C_{-\kappa\downarrow} C_{\kappa\uparrow}$$

The notation is fairly obvious. The chemical potential that appears may be thought of as a potential, $-\mu$, that arises from a uniform background of positive charge. When no interactions are present (when A = 0), the Hamiltonian achieves its minimum for the state $\prod_{\varepsilon^\circ(k) \leq \mu} C_{k\uparrow}^+ C_{-k\downarrow}^+ |0\rangle$, where $|0\rangle$ is the mathematical vacuum, and the energy of the state is, of course, proportional to the volume of the system. We now show that even when interactions are included, the ground state energy of the Hamiltonian is no greater, in the limit of infinite volume, than the ground state energy when interactions are absent.

From the fact that the ground state energy can be defined by a variational principle it follows that,

(1) E(ground state) $\leq \langle$normal/$H_o + H_{int}$/normal$\rangle$ =

E(normal) + $\langle$normal/H_{int}/normal$\rangle$

On the other hand, we have E(ground state) = minimum ($H_o + H_{int}$), so that E(ground state) $\geq$ minimum (H_o) + minimum (H_{int}). But the last term is clearly positive, so that

(2) E(ground state) $\geq$ E(normal)

However, in (1) the last term is independent of volume, so that in the limit of infinite volume, combining (1) with (2), we have

E(normal) $\geq$ E(ground state) $\geq$ E(normal), which is the equality we sought to demonstrate.

Thus the correlated state, if chosen to be the vacuum state, cannot be stable. Nevertheless, nothing prevents us from studying an unstable vacuum. The very same methods one uses to derive the gap equation and Bogoliubov-Valatin operators for attractive interactions can be used for repulsive interactions as well. In fact, while the gap equation in both cases is identical, the B-V operators are slightly different. Attractive interaction yields as operators:

$$\gamma_{k\uparrow}^{+} = [2\omega_k]^{-1/2}\left[(\omega_k + \mathcal{E}_k)^{1/2} c_{k\uparrow}^{+} + (\omega_k - \mathcal{E}_k)^{1/2} c_{-k\downarrow}\right]$$

$$\gamma_{-k\downarrow} = [2\omega_k]^{-1/2}\left[(\omega_k + \mathcal{E}_k)^{1/2} c_{-k\downarrow} - (\omega_k - \mathcal{E}_k)^{1/2} c_{k\uparrow}^{+}\right]$$

and their adjoints. In our notation $\omega_k^2 = \mathcal{E}_k^2 + \Delta_k^2$, Δ_k is the gap, $\mathcal{E}_k = \mathcal{E}_k^\circ - \mu$, and $|\mathcal{E}_k|$ is constrained to be less than δ. For repulsive interactions the "names" of these operators are interchanged. The first operator becomes $\gamma_{-k\downarrow}$ and the second becomes $\gamma_{k\uparrow}^{+}$. Whereas the Hamiltonian for attractive interactions takes the form

$$\sum_{|\mathcal{E}_k|>\delta} \mathcal{E}_k\left[c_{k\uparrow}^{+} c_{k\uparrow} + c_{-k\downarrow}^{+} c_{-k\downarrow}\right] + \sum \Big[\Big\{(\mathcal{E}_k - \omega_k) + \frac{1}{2}\frac{\Delta_k^2}{\omega_k}\Big\} + \omega_k\left\{\gamma_{k\uparrow}^{+}\gamma_{k\uparrow} + \gamma_{-k\downarrow}^{+}\gamma_{-k\downarrow}\right\} + \text{terms in } \frac{1}{V}\Big]$$

for repulsive interaction the sum over $|\mathcal{E}_k| \leq \delta$ becomes

$$\sum \Big[\Big\{(\mathcal{E}_k + \omega_k) + \frac{1}{2}\frac{\Delta_k^2}{\omega_k} - \omega_k\left\{\gamma_{k\uparrow}^{+}\gamma_{k\uparrow} + \gamma_{-k\downarrow}^{+}\gamma_{-k\downarrow}\right\} + \text{terms in } \frac{1}{V}\Big]$$

In both cases the physical vacuum is defined as

$$|G\rangle = \prod_{|\mathcal{E}_k| \leq \delta} \gamma_{k\uparrow}\gamma_{-k\downarrow} \prod_{\mathcal{E}_k < -\delta} c_{k\uparrow}^{+} c_{-k\downarrow}^{+} |0\rangle$$

but in each case $\gamma_{k\uparrow}$ and $\gamma_{-k\downarrow}$ are defined differently. The Hamiltonian with the $\frac{1}{V}$ terms neglected will suffice when applied to states that involve only a finite number of excitations out of the ground state. For states involving an infinite number of excitations these terms cannot be dropped. Thus without these terms it would appear that by exciting all the "particles", the energy of the correlated state for repulsive interactions could drop in energy from $\sum\left[(\mathcal{E}_k + \omega_k) + \frac{1}{2}\frac{\Delta_k^2}{\omega_k}\right]$ to $\sum(\mathcal{E}_k - \omega_k) + \frac{1}{2}\frac{\Delta_k^2}{\omega_k}$, -- the energy of the ground state for attractive interactions! The $\frac{1}{V}$ terms prevent this, and the energy cannot be dropped below that of the normal state.

Thus we see that while a correlated "gap" state exists for repulsive interactions, such asstate is unstable against collapse to the normal state. But this applies only to the BCS reduced Hamiltonian. For the electron gas, for example, we know that the ground state is not the normal state but a correlated state. The correlation of this state is such that electrons are bound to holes in pairs, and each pair has a binding energy roughly equal to the plasma energy. While in an extremely crude way this energy may be claimed to be a gap energy, and the ground state consequently a "gap" state, the presence of other excitations with vanishingly small energy rob this"gap" of any real meaning.

(1) J. Bardeen, L. Cooper, and J. Schrieffer, Phys. Rev. 108, 1175 (1957).

(2) J. Osada, Y. Hama, and D. M. Redondo, Nuovo Cimento, 28, 1337 (1963).